

Structure 5b

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

```
=> d que l1;d que l2
```

```
00          44 SEA FILE=REGISTRY ABB=ON   PLU=ON   NSC3-N3C3/ES
```

L2 4 SEA FILE=REGISTRY ABB=ON PLU=ON 333.1144/RID

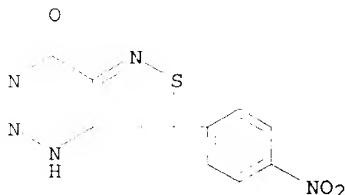
=> d 12 ide can 1-4

By more match
cleaned streets

```

L2 ANSWER 1 OF 4  REGISTRY  COPYRIGHT 2002 ACS
RN 72633-09-1  REGISTRY
CN Isothiazolo[4,3-d]-1,2,3-triazin-4(1H)-one, 7-(4-nitrophenyl)- (9CI)  (CA
INDEX NAME)
FS 3D CONCORD
MF C10 H5 N5 O3 S
LC STN Files:  BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

```



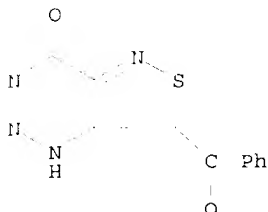
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 92:76382

L2 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2002 ACS

RN 72632-96-3 REGISTRY
 CN Isothiazolo[4,3-d]-1,2,3-triazin-4(1H)-one, 7-benzoyl- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C11 H6 N4 O2 S
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
 (*File contains numerically searchable property data)

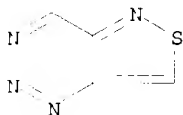


PROPEFTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 92:76382

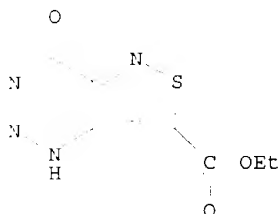
L2 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2002 ACS
 RN 55402-82-9 REGISTRY
 CN Isothiazolo[4,3-d]-1,2,3-triazine (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C4 H2 N4 S
 CI RPS



PROPEFTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2002 ACS
 RN 54968-80-8 REGISTRY
 CN Isothiazolo[4,3-d]-1,2,3-triazine-7-carboxylic acid, 1,4-dihydro-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C7 H6 N4 O3 S
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
 (*File contains numerically searchable property data)

Handwritten notes:
 1929
 1929
 1929



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 92:76382

REFERENCE 2: 82:139991

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 10:47:16 ON 16 SEP 2002

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 16 Sep 2002 VOL 137 ISS 12

FILE LAST UPDATED: 15 Sep 2002 (20020915/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> s l2

L3 2 L2

=> d .ca 1-2

L3 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1980:76382 HCAPLUS

DOCUMENT NUMBER: 92:76382
 TITLE Synthesis and reactions of 4-aminoisothiazoles
 AUTHOR(S): Gewald, Karl; Bellmann, Peter
 CORPORATE SOURCE: Sekt. Chem., Tech. Univ. Dresden, Dresden, DDR-8027,
 Ger. Dem. Rep.
 SOURCE Liebigs Ann. Chem. (1979), (10), 1534-46
 CODEN: LACHDL
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 AB 4-MeC6H4ON:CRCN (R = CONH2, CO2Et, CPh, Ph, 4-O2NC6H4) reacted with
 R1CH2SH (R1 = CPh, CO2Et, COMe, CO2H, C6H4NO2-4, CHO, Ph) to give the
 corresponding aminoisothiazoles I via the intermediates R1CH2SN:CRCN.
 Decarboxylation gave 5-unsubstituted 4-aminoisothiazoles, e.g., reaction
 of I (R = CONH2, R1 = CO2Et) with HCl gave 3-carboxy-4-aminoisothiazole,
 which was heated with Ac2O to give 4-acetamidoisothiazole. I were also
 converted into the ring systems II (R1 = CPh, CO2Et, C6H4NO2-4), III (R1
 = CO2Et, COMe), IV (R = CONH2, Ph, C6H4NO2-4), and V (R = CONH2, CO2Et; R2
 = H, Me).
 CC 18-7 (Heterocyclic Compounds (More Than One Hetero Atom))
 IT 54968-79-5P **54968-80-8P** 72632-83-8P 72632-86-1P
 72632-88-3P 72632-91-8P 72632-92-9P 72632-93-0P 72632-94-1P
 72632-95-2P **72632-96-3P** 72632-97-4P 72632-98-5P
 72632-99-6P 72633-00-2P 72633-01-3P 72633-02-4P 72633-03-5P
 72633-04-6P 72633-05-7P 72633-06-8P 72633-08-0P **72633-09-1P**
 FL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

L3 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1975:139991 HCAPLUS
 DOCUMENT NUMBER: 82:139991
 TITLE: New synthesis of 4-aminoisothiazoles
 AUTHOR(S): Gewald, Karl; Bellmann, Peter; Jaensch, Hans J.
 CORPORATE SOURCE: Sekt. Chem., Tech. Univ. Dresden, Dresden, E. Ger.
 SOURCE Z. Chem. (1975), 15(1), 18-19
 CODEN: ZECCAL
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 AB Aminoisothiazoles I (R = CONH2, CO2Et; R1 = CO2Et, Ac) were prepd. in 48
 60% yield by treating NCCR:NO3SC6H4Me-p with R1CH2SH in the presence of
 base at <40.degree.. H2NCOC(CN):NSCH2CO2Et was also isolated and
 diazotized, giving the isothiazolotriazinone II (X = N). Condensation of
 I (R = CONH2, R1 = CO2Et) with HC(OEt)3 gave II (X = CH).
 CC 18-7 (Heterocyclic Compounds (More Than One Hetero Atom))
 IT 54968-75-1P 54968-76-2P 54968-79-5P **54968-80-8P**
 FL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)